

A short analysis of chemical bonds.

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Abstract: Nothing prohibits to give a definition of the multiplicity of bond: the multiplicity of bond is the energy of bond expressed in dimensionless units. It is easy to show, that relation $\text{multiplicity} = f(L)$ and $E = f(L)$, where multiplicity is multiplicity of bond, L – length of bond in Å, E – energy of bond in kJ/mole will be described by function $y = a + b/x + c/x^2$ for any types of bond (C-N, C-O, C-S, N-N, N-O, O-O, C-P).

Keywords: chemical bond, bond energy, bond multiplicity, function.

RESULTS AND DISCUSSION.

We'll find the dependence $\text{Multiplicity} = f(L)$ and $E = f(L)$ using function $y = a + b/x + c/x^2$ for C-O bonds, where the multiplicity — is multiplicity of bond, L – length of bond in Å, E – energy of bond in kJ/mole.

For the length of bonds let us take the findings:

$$\text{H}_3\text{C}-\text{OH} \quad L_{\text{C-O}} = 1.434 \text{ Å} \quad (6) \quad \text{Multiplicity} = 1$$

$$\text{H}_2\text{C}=\text{O} \quad L_{\text{C-O}} = 1.206 \text{ Å} \quad (6) \quad \text{Multiplicity} = 2$$

$$\text{C}\equiv\text{O} \quad L_{\text{C-O}} = 1.12823 \text{ Å} \quad (7) \quad \text{Multiplicity} = 3$$

$$y = a + b/x + c/x^2 \quad X = 1/x \quad Y = \frac{(y - y_1)}{(1/x - 1/x_1)}$$

$$b_1 = b + c/x_1 \quad Y = b_1 + cX$$

$$c = \frac{(\sum (1/x \cdot Y) - (\sum (1/x) \cdot \sum Y)/n)}{((\sum 1/x^2) - (\sum (1/x))^2/n)}$$

$$b_1 = (\sum Y)/n - c(\sum (1/x))/n$$

n —the number of given value Y .

Let us find a from the equality: $\sum y = na + b\sum(1/x) + c\sum(1/x^2)$, when $n = 3$

Table 1. Calculation of ratios for relation Multiplicity = f(L) for C-O bond.

	1/x	1/x ²	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	x (L, Å)	y (multiplicity)
	0.82918740	0.68755174	7.58510526	6.28947368	1.43400	1
	0.88634410	0.78560586	10.58234503	9.37959905	1.20600	2
					1.12823	3
Σ	1.71553149	1.47315760	18.16745029	15.66907273	3.76823	6

$$1/x_1 = 0.69735007$$

$$x_1 = 1.43400$$

$$y_1 = 1$$

$$\Sigma(1/x^2) = 1.95945472$$

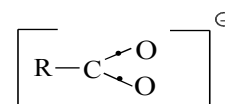
$$\Sigma(1/x) = 2.41288156$$

$$c = 52.43899244$$

$$b = -72.46498138$$

$$a = 26.03252883$$

$$\text{Multiplicity (C-O)} = 26.03252883 - \frac{72.46498138}{L} + \frac{52.43899244}{L^2}$$

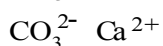


Let us calculate from the equation:

$$\text{HCOO}^\ominus \text{Na}^\oplus \quad \text{Lc-o} = 1.27 \text{ Å} \quad (8) \quad \text{Multiplicity (L=1.27 Å)} = 1.486$$

$$\text{NH}_3^\oplus \text{CH}_2\text{COO}^\ominus \quad \text{Lc-o} = 1.26 \text{ Å} \quad (8) \quad \text{Multiplicity (L=1.26 Å)} = 1.551$$

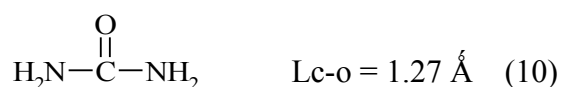
$$\text{CO}_3^{2-} \text{K}_2^{2+} 3\text{H}_2\text{O} \quad \text{Lc-o} = 1.29 \text{ Å} \quad (9) \quad \text{Multiplicity (Lc-o} = 1.29 \text{ Å)} = 1.370$$



$$\text{O}=\text{CO} \quad \text{Lc-o} = 1.162 \text{ Å} \quad (4) \quad \text{Multiplicity (Lc-o} = 1.162 \text{ Å)} = 2.507$$

So as we see, as expected theory of three-electrone bond, frequency of C-O bond in carboxylate anion is equal to 1.5. In carbonate anion frequency of C-O is equal to 1.37, while the carbon dioxide is equal to 2.5, which correlates well with the classical ideas.

In urea C-O multiplicity of bonds equal to about 1.5, and C-N is approximately 1.7 (as shown below).



$$\text{Multiplicity (Lc-o} = 1.27 \text{ Å)} = 1.486 \approx 1.5 \quad \text{Multiplicity C-N} = 1.686$$

Now let's find the dependence $E = f(L)$ для C–O bonds.

For the bonds energy let's take the data:

$$\text{C–O} \quad L_{\text{C–O}} = 1.434 \text{ \AA} \quad E_{\text{C–O}} = 351.708 \text{ kJ/mole} \quad (2)$$

$$\text{C=O (for H}_2\text{C=O)} \quad L_{\text{C=O}} = 1.206 \text{ \AA} \quad E_{\text{C=O}} = 686.668 \text{ kJ/mole} \quad (2)$$

$$\text{C}\equiv\text{O} \quad L_{\text{C}\equiv\text{O}} = 1.12823 \text{ \AA} \quad E_{\text{C}\equiv\text{O}} = 1071.773 \text{ kJ/mole} \quad (7)$$

Table 2. Calculation factors for dependency $E = f(L)$ for C–O bond.

	$1/x$	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	$x (L, \text{\AA})$	$y (E, \text{kJ/mole})$
	0.82918740	0.68755174	2540.70685895	2106.72210526	1.43400	351.708
	0.88634410	0.78560586	3809.98813722	3376.96049318	1.20600	686.668
					1.12823	1071.773
Σ	1.71553149	1.47315760	6350.69499617	5483.68259844	3.76823	2110.149

$$1/x_1 = 0.69735007 \quad x_1 = 1.43400 \quad y_1 = 351.708$$

$$\Sigma(1/x^2) = 1.95945472 \quad \Sigma(1/x) = 2.41288156$$

$$c = 22207.04265404 \quad b = -31359.17576343 \quad a = 11420.81052442$$

$$E_{\text{C–O}} = 11420.81052442 - \frac{31359.17576343}{L} + \frac{22207.04265404}{L^2}$$

Let us find from the equation:

$$E (L = 1.434 \text{ \AA}) = 351.708 \text{ kJ/mole}$$

$$E (L = 1.206 \text{ \AA}) = 686.668 \text{ kJ/mole}$$

$$E (L = 1.12823 \text{ \AA}) = 1072.542 \text{ kJ/mole}$$

$$\text{O=CO} \quad L_{\text{C–O}} = 1.16213 \text{ \AA} \quad (29)$$

$$E (L = 1.16213 \text{ \AA}) = 879.596 \text{ kJ/mole} = 210.088 \text{ kcal/mole}$$

$$\text{O=CO} \quad L_{\text{C–O}} = 1.162 \text{ \AA} \quad E (\text{average}) = 192 \text{ kcal/mole} \quad D = 127 \text{ kcal/mole} \quad (11)$$

$$E (L = 1.162 \text{ \AA}) = 880.257 \text{ kJ/mole} = 210.246 \text{ kcal/mole}$$

$$\text{NH}_3^+ \text{—CH}_2\text{COO}^- \quad L_{\text{C–O}} = 1.26 \text{ \AA} \quad E (L = 1.26 \text{ \AA}) = 520.383 \text{ kJ/mole}$$

$$\text{HCO-OH} \quad L_{\text{C-O}} = 1.41 \text{ \AA} \quad D \sim 90 \text{ kcal/mole} \quad (4)$$

$$E(L = 1.41 \text{ \AA}) = 350.243 \text{ kJ/mole} = 83.654 \text{ kcal/mole}$$

$$\text{H}_3\text{C-OH} \quad L_{\text{C-O}} = 1.434 \text{ \AA} \quad D \sim 90 \text{ kcal/mole} \quad (4)$$

$$E(L = 1.434 \text{ \AA}) = 351.708 \text{ kJ/mole} = 84.004 \text{ kcal/mole}$$

$$\text{CH}_3\text{CO-OH} \quad L_{\text{C-O}} = 1.43 \text{ \AA} \quad D \sim 90 \text{ kcal/mole} \quad (4)$$

$$E(L = 1.430 \text{ \AA}) = 351.038 \text{ kJ/mole} = 83.844 \text{ kcal/mole}$$

So we can see the binding energy calculated from the equation for C-O bond nice correlated with experimental data.

We'll find the dependence Multiplicity = $f(L)$ and $E = f(L)$ for C-N bonds.

For the bonds energy let's take the data (2):

$$\text{C-N} \quad E = 291.834 \text{ kJ/mole}$$

$$\text{C=N} \quad E = 615.489 \text{ kJ/mole}$$

$$\text{C}\equiv\text{N (for HC}\equiv\text{N)} \quad E = 866.709 \text{ kJ/mole}$$

For lengths of bonds let us take the data:

$$\text{CH}_3\text{-NH}_2 \quad (L_{\text{C-N}} = 1.4714 \text{ \AA}) \quad (12)$$

$$\text{HC}\equiv\text{N} \quad (L_{\text{C}\equiv\text{N}} = 1.157 \text{ \AA}) \quad (6)$$

$$\text{C=N} \quad (L_{\text{C=N}} = 1.28 \text{ \AA}) \quad (14)$$

We'll find the dependence Multiplicity = $f(L)$

Table 3. Calculation coefficients for dependence Multiplicity = $f(L)$ for C-N bond.

	$1/x$	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	$x (L, \text{\AA})$	$y (\text{Multiplicity})$
	0.78125000	0.61035156	9.84008359	7.68756531	1.4714	1
	0.86430424	0.74702181	10.82957888	9.36005089	1.2800	2
					1.1570	3
Σ	1.64555424	1.35737337	20.66966247	17.04761620	3.9084	6

$$1/x_1 = 0.67962485$$

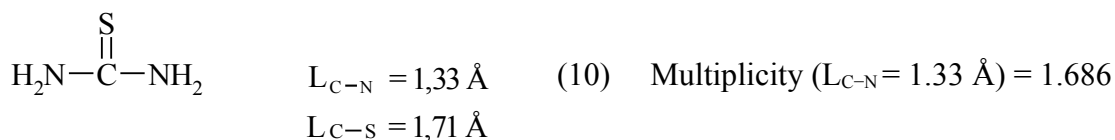
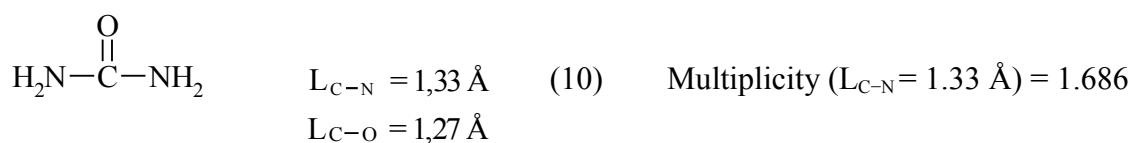
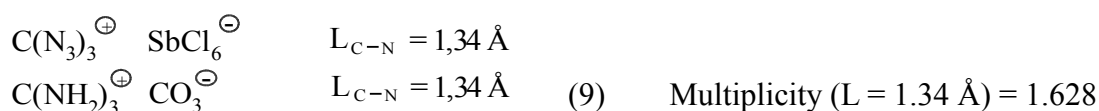
$$x_1 = 1.4714$$

$$y_1 = 1$$

$$\begin{aligned}\Sigma(1/x^2) &= 1.81926331 & \Sigma(1/x) &= 2.32517908 \\ c &= 11.91384503 & b &= -7.56455294 & a &= 0.63817306\end{aligned}$$

$$\text{Multiplicity (C-N)} = 0.63817306 - \frac{7.56455294}{L} + \frac{11.91384503}{L^2}$$

Let us find from the equation:



We'll find the dependence $E = f(L)$ for C-N bonds.

Table 4. Calculation coefficients for dependence $E = f(L)$ for C-N bond.

	$1/x$	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	$x \text{ (L, \AA)}$	$y \text{ (E, kJ/mole)}$
	0.78125000	0.61035156	3184.79225580	2488.11894984	1.4714	291.834
	0.86430424	0.74702181	3112.82707944	2690.42962786	1.2800	615.489
					1.1570	866.709
Σ	1.64555424	1.35737337	6297.61933524	5178.54857771	3.9084	1774.032

$$\begin{aligned}1/x_1 &= 0.67962485 & x_1 &= 1.4714 & y_1 &= 291.834 \\ \Sigma(1/x^2) &= 1.81926331 & \Sigma(1/x) &= 2.32517908 \\ c &= -866.48412671 & b &= 4450.61712191 & a &= -2332.69568587\end{aligned}$$

$$E(\text{C-N}) = -2332.69568587 + \frac{4450.61712191}{L} - \frac{866.48412671}{L^2}$$

$$E(L = 1.33 \text{ \AA}) = 523.790 \text{ kJ/mole}$$

We'll find the dependence Multiplicity = f(L) and E = f(L) for C-S bonds. Firstly we'll find the dependence Multiplicity = f(L).

For lengths of bonds let us take the date:

$$\text{H}_3\text{C-SH} \quad \text{Multiplicity} = 1 \quad L = 1.818 \text{ \AA} \quad (15)$$

$$\text{H}_2\text{C=S} \quad \text{Multiplicity} = 2 \quad L = 1.6108 \text{ \AA} \quad (16)$$

$$\text{C}\equiv\text{S} \quad \text{Multiplicity} = 3 \quad L = 1.53492 \text{ \AA} \quad (7)$$

In the molecule CS multiplicity equal to 3, what confirming the spectral data of the compounds CS, HCP, CP (7), (17), namely the frequency of fluctuations and constant anharmonicity (ω_{exe}), what for $\text{C}\equiv\text{P}$ and $\text{C}\equiv\text{S}$ bond are almost identical:

$$\begin{array}{llll} \text{CS} & L_{\text{C-S}} = 1.53492 \text{ \AA} & D = 169.6 \text{ kcal/mole} & \omega_e = 1285.08 \text{ cm}^{-1} \\ & & & \omega_{\text{exe}} = 6.46 \text{ cm}^{-1} \end{array}$$

$$\begin{array}{llll} \text{CP} & L_{\text{C-P}} = 1.5583 \text{ \AA} & D = 122 \text{ kcal/mole} & \omega_e = 1239.67 \text{ cm}^{-1} \\ & & & \omega_{\text{exe}} = 6.86 \text{ cm}^{-1} \end{array}$$

$$\begin{array}{llll} \text{H-C}\equiv\text{P} & L_{\text{C-P}} = 1.5421 \text{ \AA} & & \nu_1 = 3216.9 \text{ cm}^{-1} \\ & L_{\text{C-H}} = 1.0667 \text{ \AA} & & \nu_2 = 1278.4 \text{ cm}^{-1} \\ & & & \nu_3 = 674.7 \text{ cm}^{-1} \end{array}$$

Table 5. Calculation coefficients for dependence Multiplicity = f(L) for C-S bond.

	$1/x$	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	x (L, \AA)	y (Multiplicity)
	0.62080954	0.38540448	14.13337066	8.77413127	1.81800	1
	0.65149975	0.42445193	19.71516575	12.84442560	1.61080	2
					1.53492	3
Σ	1.27230929	0.80985641	33.84853640	21.61855688	4.96372	6

$$1/x_1 = 0.55005501 \quad x_1 = 1.81800 \quad y_1 = 1$$

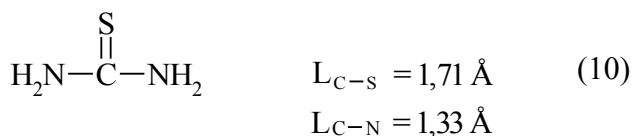
$$\Sigma(1/x^2) = 1.11241692 \quad \Sigma(1/x) = 1.82236429$$

$$c = 181.87538814 \quad b = -198.81807222 \quad a = 55.33256579$$

$$\text{Multiplicity (C-S)} = 55.33256579 - \frac{198.81807222}{L} + \frac{181.87538814}{L^2}$$

Let us find from the equation:

$$\text{CS}_3^{2-} \quad L_{\text{C-S}} = 1,71 \text{ \AA} \quad (9) \quad \text{Multiplicity (Lc-s} = 1.71 \text{ \AA}) = 1.263$$



$$\text{Multiplicity (C-S)} = 1.263 \quad \text{Multiplicity (C-N)} = 1.686$$

$$\text{S=C=S} \quad L_{\text{C-S}} = 1.5529 \text{ \AA} \quad (17)$$

$$\text{Multiplicity (Lc-s} = 1.5529 \text{ \AA}) = 2.722$$

In general, we see that oxygen sulfur analogs behave quite as expected:

- thiourea and thiocarbonates anion have slightly lowered frequency of C-S bond (compared to the C-O) (1.263 to 1.507, and 1.263 to 1.370), due to more efficient delocalization of electrons on the sulfur atom is greater (compared to an oxygen atom)
- carbon disulfide compared with carbon dioxide multiplicity of C-S bond slightly higher than the frequency of the C-O bond (2.7 against 2.5 in carbon dioxide) that can be explained by coupling undivided pair of electrons sulfur and oxygen with a double bond and therefore more coupling in the case of sulfur atom.

We'll find the dependence $E = f(L)$ for C-S bonds.

For energies of bonds let us take the data:

$$\text{C-S} \quad L = 1.818 \text{ \AA} \quad E = 259.594 \text{ kJ/mole} \quad (2)$$

$$\text{C=S} \quad L = 1.6108 \text{ \AA} \quad E = 728.538 \text{ kJ/mole} \quad (2)$$

$$\text{C}\equiv\text{S} \quad L = 1.53492 \text{ \AA} \quad E = 709.606 \text{ kJ/mole} \quad (7)$$

Table 6. Calculation coefficients for dependence $E = f(L)$ for C-S bond.

	$1/x$	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	$x (L, \text{\AA})$	$y (E, \text{kJ/mole})$
	0.62080954 0.65149975	0.38540448 0.42445193	6627.75936908 4436.03058434	4114.57621622 2890.07282747	1.81800 1.61080 1.53492	259.594 728.538 709.606
Σ	1.27230929	0.80985641	11063.78995342	7004.64904369	4.96372	1697.738

$$1/x_1 = 0.55005501 \quad x_1 = 1.81800 \quad y_1 = 259.594$$

$$\Sigma(1/x^2) = 1.11241692 \quad \Sigma(1/x) = 1.82236429$$

$$c = -71414.57485742 \quad b = 90244.55278987 \quad a = -27772.64385690$$

$$E_{c-s} = -27772.64385690 + \frac{90244.55278987}{L} - \frac{71414.57485742}{L^2}$$

Let us find from the equation:

$$SC=S \quad L_{c-s} = 1.5529 \text{ \AA} \quad E(L = 1.5529 \text{ \AA}) = 726.729 \text{ kJ/mole} = 173.576 \text{ kcal/mole}$$

$$E_{c-s} (\text{average}) = 128 \text{ kcal/mole} \quad (11)$$

We'll find the dependence Multiplicity = $f(L)$ and $E = f(L)$ for N-N bonds.

For energies of bonds let us take the date:

$$N-N \quad E = 160.781 \text{ kJ/mole} \quad (2)$$

$$N=N \quad E = 418.000 \text{ kJ/mole} \quad (40)$$

$$N \equiv N \quad E = 945.333 \text{ kJ/mole} \quad (18)$$

For lengths of bonds let us take the date:

$$H_2N-NH_2 \quad L = 1.4530 \text{ \AA} \quad (26)$$

$$HN=NH \quad L = 1.2300 \text{ \AA} \quad (27)$$

$$N \equiv N \quad L = 1.0976 \text{ \AA} \quad (28)$$

Firstly we'll find the dependence Multiplicity = $f(L)$

Table 7. Calculation coefficients for dependence Multiplicity = $f(L)$ for N-N bond.

	$1/x$	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	$x (L, \text{\AA})$	$y (\text{Multiplicity})$
	0.81300813 0.91107872	0.66098222 0.83006443	8.01430493 8.97474845	6.51569507 8.17670231	1.4530 1.2300 1.0976	1 2 3
Σ	1.72408685	1.49104665	16.98905339	14.69239737	3.7806	6

$$\begin{aligned}
1/x_1 &= 0.68823125 & x_1 &= 1.4530 & y_1 &= 1 \\
\Sigma(1/x^2) &= 1.96470890 & \Sigma(1/x) &= 2.41231809 \\
c &= 9.79339013 & b &= -6.68791795 & a &= 0.96407492
\end{aligned}$$

$$\text{Multiplicity (N-N)} = 0.96407492 - \frac{6.68791795}{L} + \frac{9.79339013}{L^2}$$

We'll find the dependence $E = f(L)$ for N-N bonds.

Table 8. Calculation coefficients for dependence $E = f(L)$ for N-N bond.

	$1/x$	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	$x (L, \text{\AA})$	$y (E, \text{kJ/mole})$
	0.81300813	0.66098222	2061.43150049	1675.96056951	1.4530	160.781
	0.91107872	0.83006443	3520.57842393	3207.52407428	1.2300	418.000
					1.0976	945.333
Σ	1.72408685	1.49104665	5582.00992443	4883.48464379	3.7806	1524.114

$$\begin{aligned}
1/x_1 &= 0.68823125 & x_1 &= 1.4530 & y_1 &= 160.781 \\
\Sigma(1/x^2) &= 1.96470890 & \Sigma(1/x) &= 2.41231809 \\
c &= 14878.53765631 & b &= -20274.81508318 & a &= 7067.14065437
\end{aligned}$$

$$E (\text{N-N}) = 7067.14065437 - \frac{20274.81508318}{L} + \frac{14878.53765631}{L^2}$$

Let us find from the equation:

$$\begin{aligned}
\text{N}_2^{\oplus} \quad L &= 1,116 \text{ \AA}, \quad \text{Multiplicity} = 2.835, \quad E = 846.001 \text{ kJ/mole} \\
\text{experimentally found} \quad E &= 843.26 \text{ kJ/mole} \quad (19)
\end{aligned}$$

As we see in the latter case are almost the same value of energy of equation identified and obtained experimentally.

We'll find the dependence $\text{Multiplicity} = f(L)$ for N-O bonds.

For lengths of bonds let us take the date:

$$\begin{aligned}
\text{NH}_2\text{—OH} \quad L_{\text{N-O}} &= 1,453 \text{ \AA} & (20) & \quad \text{Multiplicity} = 1 \\
\text{CH}_3\text{—NO}_2 \quad L_{\text{N-O}} &= 1,224 \text{ \AA} & (12) & \quad \text{Multiplicity} = 1.5 \\
\text{NO} \quad L_{\text{N-O}} &= 1,1507 \text{ \AA} & (19) & \quad \text{Multiplicity} = 2.5
\end{aligned}$$

Table 9. Calculation coefficients for dependence Multiplicity = f (L) for N-O bond.

	$1/x$	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	x (L, Å)	y (Multiplicity)
	0.81699346	0.66747832	3.88312664	3.17248908	1.4530	1.0
	0.86903624	0.75522398	8.29623106	7.20972544	1.2240	1.5
					1.1507	2.5
Σ	1.68602970	1.42270230	12.17935770	10.38221452	3.8277	5.0

$$1/x_1 = 0.68823125 \quad x_1 = 1.4530 \quad y_1 = 1.0$$

$$\Sigma(1/x^2) = 1.89636455 \quad \Sigma(1/x) = 2.37426095$$

$$c = 84.79763896 \quad b = -123.75637485 \quad a = 46.00756377$$

$$\text{Multiplicity (N-O)} = 46.00756377 - \frac{123.75637485}{L} + \frac{84.79763896}{L^2}$$

$$\text{N}_2\text{O} \quad \text{N-N} = 1.1282 \text{ Å} \quad (30)$$

$$\text{N-O} = 1.1843 \text{ Å}$$

$$\text{Multiplicity (N-O)} (L = 1.1843 \text{ Å}) = 1.969 \approx 1.97$$

$$\text{Multiplicity (N-N)} (L = 1.1282 \text{ Å}) = 2.730$$

$$\text{NO}_3^- \quad L(\text{N-O}) = 1.243 \text{ Å} \quad (31)$$

$$\text{Multiplicity} (L = 1.243 \text{ Å}) = 1.328 \approx 1.33$$

We'll find the dependence $E = f(L)$ for N-O bond.

For energies of bonds let us take the data:

$$\text{N-O} \quad E = 221.900 \text{ kJ/mole} \quad (22)$$

$$\text{N=O} \quad E = 607.086 \text{ kJ/mole} \quad (22)$$

$$\text{NO} \quad L = 1.15070 \text{ Å} \quad E = 626.847 \text{ kJ/mole} \quad (19)$$

$$\text{N-O} \quad L = 1.453 \text{ Å} \quad (\text{NH}_2\text{-OH}) \quad (20)$$

Lengths L when N=O Multiplicity = 2 calculated by the formula:

$$\text{Multiplicity (N-O)} = 46.00756377 - \frac{123.75637485}{L} + \frac{84.79763896}{L^2}$$

$$2 = 46.00756377 - \frac{123.75637485}{L} + \frac{84.79763896}{L^2}$$

$$44.00756377 L^2 - 123.75637485 L + 84.79763896 = 0$$

$$L = 1.18208253 \text{ \AA}$$

The value of $L = 1.63007893 \text{ \AA}$ is not considered as the basis of bond lengths, it is clear that this multiplicity <1.

So,	N=O	Multiplicity = 2	$L = 1.18208253 \text{ \AA}$
N-O	$L = 1.453 \text{ \AA}$		$E = 221.900 \text{ kJ/mole}$
N=O	$L = 1.18208253 \text{ \AA}$		$E = 607.086 \text{ kJ/mole}$
NO	$L = 1.1507 \text{ \AA}$		$E = 626.847 \text{ kJ/mole}$

Table 10. Calculation coefficients for dependence $E = f(L)$ for N-O bond.

	$1/x$	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	$x (L, \text{\AA})$	$y (E, \text{kJ/mole})$
	0.84596462	0.71565614	2442.00695125	2065.85148606	1.45300000	221.900
	0.86903624	0.75522398	2239.68925320	1946.37112471	1.18208253	607.086
					1.15070000	626.847
Σ	1.71500086	1.47088013	4681.69620445	4012.22261077	3.78578253	1455.833

$$1/x_1 = 0.68823125 \quad x_1 = 1.4530 \quad y_1 = 221.900$$

$$\Sigma(1/x^2) = 1.94454237 \quad \Sigma(1/x) = 2.40323211$$

$$c = -8769.11638979 \quad b = 15895.54907490 \quad a = -6564.31416262$$

$$E(\text{N-O}) = -6564.31416262 + \frac{15895.54907490}{L} - \frac{8769.11638979}{L^2}$$

Let us find from the equation:

$$\text{CH}_3\text{—NO}_2 \quad L_{\text{N-O}} = 1.224 \text{ \AA} \quad E(L = 1.224 \text{ \AA}) = 569.050 \text{ kJ/mole}$$

We'll find the dependence Multiplicity = $f(L)$ for C-P bond.

$$\text{H}_2\text{P—CH}_3 \quad L_{\text{C-P}} = 1.858 \text{ \AA} \quad (23) \quad \text{Multiplicity} = 1$$

$$\begin{array}{lll}
 (\text{CH}_3)_3\text{P}=\text{CH}_2 & L_{\text{C}=\text{P}} = 1.640 \text{ \AA} & (24) \quad \text{Multiplicity} = 2 \\
 \text{H}-\text{C}\equiv\text{P} & L_{\text{C}\equiv\text{P}} = 1.5421 \text{ \AA} & (17), (25) \quad \text{Multiplicity} = 3 \\
 & L_{\text{C}\equiv\text{P}} = 1.54 \text{ \AA} & (25) \\
 & L_{\text{C}\equiv\text{P}} = 1.5421 \text{ \AA} & (17)
 \end{array}$$

Table 11. Calculation coefficients for dependence Multiplicity = f(L) for C–P bond.

	$1/x$	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	$x \text{ (L, \AA)}$	$y \text{ (Multiplicity)}$
	0.60975610	0.37180250	13.97761468	8.52293578	1.8580	1
	0.64846638	0.42050864	18.14005571	11.76321621	1.6400	2
					1.5421	3
Σ	1.25822247	0.79231114	32.11767039	20.28615199	5.0401	6

$$\begin{array}{lll}
 1/x_1 = 0.53821313 & x_1 = 1.8580 & y_1 = 1 \\
 \Sigma(1/x^2) = 1.08198452 & \Sigma(1/x) = 1.79643561 & \\
 c = 107.52805439 & b = -109.46128312 & a = 28.76548555
 \end{array}$$

$$\text{Multiplicity (C-P)} = 28.76548555 - \frac{109.46128312}{L} + \frac{107.52805439}{L^2}$$

Let we see O-O bonds.

For lengths of bonds let us take the date:

$$\text{O}_3 \quad L_{\text{O-O}} = 1.2717 \text{ \AA} \quad (32)$$

$$\text{O}_2 \quad L_{\text{O-O}} = 1.20735 \text{ \AA} \quad (33)$$

$$\text{H}_2\text{O}_2 \quad L_{\text{O-O}} = 1.452 \text{ \AA} \quad (34)$$

For energies of bonds let us take the date (35)

$$\text{O}_2 = 2\text{O} \quad 119.11 \cdot 4.184 = 498.356 \text{ kJ/mole}$$

$$\text{O}_3 = \text{O}_2 + \text{O} \quad 25.6 \cdot 4.184 = 107.110 \text{ kJ/mole} - \text{this dissociation energy}$$

$$\text{O-O} \quad E = 33.2 \cdot 4.187 = 139.008 \text{ kJ/mole} \quad (2)$$

But energy O-O bond at 1.5 multiplicity we find the following manner:

$$\text{O}_3 = \text{O}_2 + \text{O} \quad 107.110 \text{ kJ/mole}$$

$$\text{O}_2 = \text{O} + \text{O} \quad 498.356 \text{ kJ/mole}$$

$$\text{O}_3 = \text{O} + \text{O} + \text{O} \quad 498.356 \text{ kJ/mole} + 107.110 \text{ kJ/mole}$$

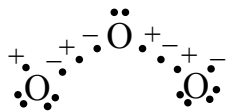
If these three oxygen atoms forming a molecule of ozone

$$\begin{array}{c} 1,5 \quad \text{O} \quad 1,5 \\ \diagdown \quad \diagup \\ \text{O} \quad \quad \text{O} \end{array}$$

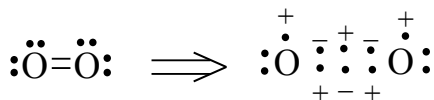
then this energy is released from the two formed three-electron bonds, so

$$\text{Fo-o when multiplicity } 1.5 = 302.733 \text{ kJ/mole} \quad 302.733 = \frac{(498.356 + 107.110)}{2}$$

HO-OH Multiplicity (O-O) = 1



Multiplicity (O-O) = 1.5



Multiplicity (O-O) = 2

Multiplicity O-O bond in the molecule of oxygen equal to 2, despite two three-electron bond as is the interaction of unpaired electrons on the oxygen atoms with three-electron bond that follows a compliance rules of octet.

H ₂ O ₂	Lo-o = 1.452 Å	Multiplicity = 1	E = 139.008 kj/mole
O ₃	Lo-o = 1.2717 Å	Multiplicity = 1.5	E = 302.733 kj/mole
O ₂	Lo-o = 1.20735 Å	Multiplicity = 2	E = 498.356 kj/mole

Table 12. Calculation coefficients for dependence Multiplicity = f (L) for O–O bond.

	1/x	1/x ²	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	x (L, Å)	y (Multiplicity)
	0.78634898	0.61834472	5.12065557	4.02662230	1.45200	1.0
	0.82826024	0.68601502	7.16563335	5.93500920	1.27170	1.5
					1.20735	2.0
Σ	1.61460922	1.30435975	12.28628893	9.96163149	3.93105	4.5

$$1/x_1 = 0.68870523 \quad x_1 = 1.452 \quad y_1 = 1.0$$

$$\Sigma(1/x^2) = 1.77867464 \qquad \Sigma(1/x) = 2.30331446$$

c = 48.79304255 b = - 66.85172754 a = 23.89786759

$$\text{Multiplicity (O-O)} = 23.89786759 - \frac{66.85172754}{L} + \frac{48.79304255}{L^2}$$

Table 13. Calculation coefficients for dependence $E = f(L)$ for O–O bond.

	$1/x$	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	$x (L, \text{\AA})$	$y (E, \text{kJ/mole})$
	0.78634898	0.61834472	1676.75866772	1318.51747088	1.45200	139.008
	0.82826024	0.68601502	2574.95601441	2132.73368486	1.27170	302.733
					1.20735	498.356
Σ	1.61460922	1.30435975	4251.71468213	3451.25115574	3.93105	940.097

$$1/x_1 = 0.68870523 \quad x_1 = 1.452 \quad y_1 = 139.008$$

$$\Sigma(1/x^2) = 1.77867464 \quad \Sigma(1/x) = 2.30331446$$

$$c = 21430.93279023 \quad b = -29935.02909385 \quad a = 10590.40848780$$

$$E (\text{O-O}) = 10590.40848780 - \frac{29935.02909385}{L} + \frac{21430.93279023}{L^2}$$

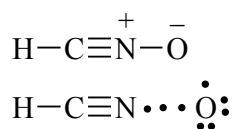
$$\text{HCNO} \quad L_{\text{C-H}} = 1.0266 \text{ \AA} \quad (36)$$

$$L_{\text{C-N}} = 1.1679 \text{ \AA}$$

$$L_{\text{N-O}} = 1.1994 \text{ \AA}$$

$$\text{Multiplicity } (L_{\text{C-N}} = 1.1679 \text{ \AA}) = 2.897$$

$$\text{Multiplicity } (L_{\text{N-O}} = 1.1994 \text{ \AA}) = 1.772$$



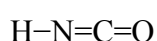
$$\text{HNCO} \quad L_{\text{H-N}} = 0.987 \text{ \AA} \quad (36)$$

$$L_{\text{N-C}} = 1.207 \text{ \AA}$$

$$L_{\text{C-O}} = 1.171 \text{ \AA}$$

$$\text{Multiplicity } (L_{\text{N-C}} = 1.207 \text{ \AA}) = 2.549$$

$$\text{Multiplicity } (L_{\text{C-O}} = 1.171 \text{ \AA}) = 2.392$$



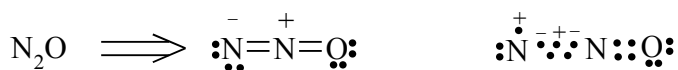
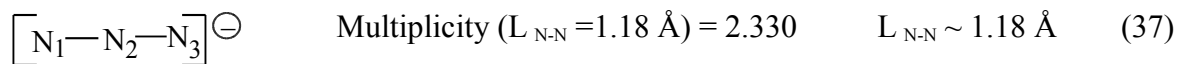
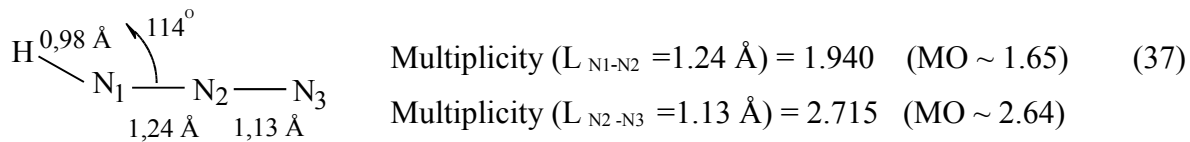
$$\text{HNCS} \quad L_{\text{H-N}} = 0.988 \text{ \AA} \quad (36) \quad \text{H}-\text{N}=\text{C}=\text{S}$$

$$L_{\text{N-C}} = 1.216 \text{ \AA}$$

$$L_{\text{C-S}} = 1.560 \text{ \AA}$$

$$\text{Multiplicity } (L_{\text{C-N}} = 1.216 \text{ \AA}) = 2.475$$

$$\text{Multiplicity } (L_{\text{C-S}} = 1.560 \text{ \AA}) = 2.620$$

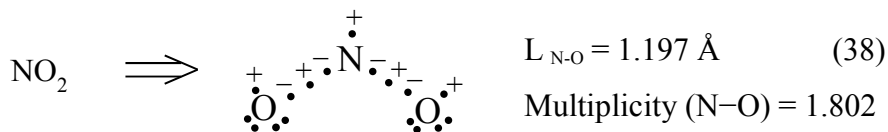


$$\text{N-N} = 1.1282 \text{ \AA} \quad (30)$$

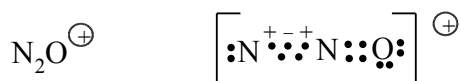
$$\text{N-O} = 1.1843 \text{ \AA}$$

$$\text{Multiplicity (L}_{\text{N-N}} = 1.1282 \text{ \AA}) = 2.730$$

$$\text{Multiplicity (L}_{\text{N-O}} = 1.1843 \text{ \AA}) = 1.969$$



$$\text{Multiplicity (N-O)} = 1.802$$

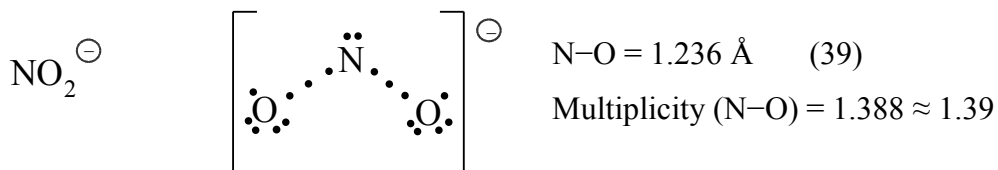


$$\text{N-N} = 1.154 \text{ \AA} \quad (30)$$

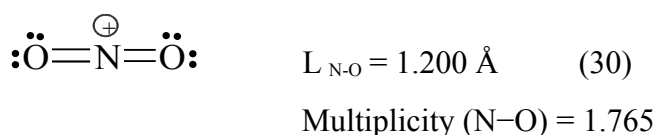
$$\text{N-O} = 1.185 \text{ \AA}$$

$$\text{Multiplicity (L}_{\text{N-N}} = 1.154 \text{ \AA}) = 2.523$$

$$\text{Multiplicity (L}_{\text{N-O}} = 1.185 \text{ \AA}) = 1.959$$



$$\text{Multiplicity (N-O)} = 1.388 \approx 1.39$$



CONCLUSION.

As exemplified in many chemical bonds (C-N, C-O, C-S, N-N, N-O, O-O) using the equation $y = a + b/x + c/x^2$ to describe the multiplicity dependence $= f(L)$ i $E = f(L)$ (where multiplicity - is multiplicity of bond, L - length of bond in Å, E - energy of bond in kJ /mole), gives good results and determine the multiplicity of power relations in many organic and inorganic compounds. In fact, to determine the multiplicity or energy of bond we can know length of the bonds must solve simple quadratic equation. Conversely, knowing the multiplicity or energy of bond can determine its length (again solving basic equation). This method is simple, but gives good results when analyzing the chemical bonds that are nice to coincide with the experimental data or other theoretical calculations.

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31. See (7), p. 218.
32. See (7), p. 130.
33. See (7), p. 46-47.
34. See (7), p. 236.
35. See (18), p. 106.
36. See (7), p. 200.
37. See (14), p. 564.
38. See (7), p. 122.
39. See (14), p. 577.
40. See (14), p. 543.